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Task Last Updated:	FY 06/10/2016
PI Name:	Xiao, Hang Ph.D.
Project Title:	Vitamins B1 and K Degradation in Spaceflight Foods: Establishment of Prediction Models and Prevention Strategies
Division Name:	Human Research
Program/Discipline:	
Program/Discipline-- Element/Subdiscipline:	HUMAN RESEARCH--Space Human Factors Engineering
Joint Agency Name:	**TechPort:** No
Human Research Program Elements:	(1) **HHC**:Human Health Countermeasures
Human Research Program Risks:	None
Space Biology Element:	None
Space Biology Cross-Element Discipline:	None
Space Biology Special Category:	None
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Zip Code:	01003-9282 **Congressional District:** 1
Comments:	
Project Type:	Ground **Solicitation / Funding Source:** 2013 HERO NNJ13ZSA002N-Crew Health (FLAGSHIP & NSBRI)
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Contact Monitor:	Douglas, Grace **Contact Phone:**
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Flight Program:	
Flight Assignment:	NOTE: Element change to Human Health Countermeasures; previously Space Human Factors & Habitability (Ed., 1/18/17)
Key Personnel Changes/Previous PI:	
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Task Description:	Currently, shelf stable foods that do not require refrigeration or freezing are the sole source of nutrition for the spaceflight crew. It is therefore crucial that these foods provide adequate nutrition to support the crew throughout the shelf life of the product. However, knowledge is currently lacking on the degradation kinetics of essential vitamins (e.g., vitamins B1 and C) during the processing and storage of spaceflight foods. To address this critical knowledge gap, this project aims to measure vitamins B1 and C degradation kinetics and use this information to establish robust computational models that are user friendly to predict vitamin stability in spaceflight foods during processing and five-years of storage. Our central hypothesis is that: (i) Based on a systematic investigation of the degradation kinetics of vitamins B1 and C, computational models can be developed to predict vitamin degradation during processing and storage of spaceflight foods. Our main approach is therefore to identify the influence of food processing, food matrix composition, storage conditions and other factors (e.g., pH) on the degradation kinetics of vitamins B1 and C. Then we will use this knowledge to establish robust models and guiding principles to predict and prevent degradation of these vitamins.

Rationale for HRP Directed Research:	
Research Impact/Earth Benefits:	A considerable amount of research has been conducted on the stability of essential vitamins including vitamins B1 and C in different food systems. However, a detailed understanding is lacking on the degradation of essential vitamins under the unique conditions experienced by spaceflight foods. The significance of the proposed research is that it will provide fundamental knowledge that is currently lacking about the roles of food processing, food matrix characteristics, and storage conditions on the degradation kinetics of vitamins B1 and C in spaceflight foods. A particularly innovative aspect of the project is that it utilizes robust mathematical modeling to simulate and predict degradation kinetics of essential vitamins. It also can help develop guiding principles to stabilize these vitamins in spaceflight foods. Successful completion of this project will provide critical information that can be used to produce more nutritious shelf stable spaceflight foods to better maintain health & wellness of spaceflight crew.
Task Progress:	Material & Methods
1. Development of modern method based on AOAC (association of analytical communities) Official Method 942.23 for vitamin B1 (Thiamine); 2. Utilization of AOAC Official Method 2012.21 for Vitamin C (Ascorbic Acid) using HPLC (high performance liquid chromatography) detection; 3. "Prediction of Isothermal Degradation by the Endpoints Method" to determine the kinetic parameters of vitamin B1 and C.

Results/Accomplishments

1. We have continued to modernize and optimize methods for sample preparation and bulk data collection, increased reproducibility and precision for thiamine detection and quantification.

• Compared to AOAC Official Method 942.2, column purification was updated to current equipment standard (Kimble Kontes FlexColumn) and current resin equivalent (Amberlite CG-50 Type I, H-form) to resin described in method. New resin and equipment demonstrated routine efficiency of >95% across tests after optimization (repeat sample addition step and repeat elution steps).

• Compared to AOAC Official Method 942.2, enzyme solution calibrated to minimize waste and still provide complete phosphorylysis of phosphate-bound thiamine in meat products. Method called for a 5% solution but was deemed more than sufficient by current research (Ndaw S. et al., 2000) and by independent testing.

• Compared to AOAC Official Method 942.2, oxidized thiamine (thiochrome) is resuspended in 4 mL isobutanol, rather than the depicted 13 mL. This is done to compensate for the change in equipment from a cuvette-style fluorescence detector to a 96-well plate reader which is more sensitive and offers higher statistical significance determination of data. The equation to calculate original concentration of thiamine still applies.

2. We have optimized the extraction efficiency, HPLC sensitivity, and ensured reproducibility for vitamin C before and after retort processing.

• Compared to AOAC Official Method 2012.12, stabilizers, TCEP hydrochloride and EDTA, were premixed prior to vitamin C extraction blend to enhance dehydroascorbic acid (DHAA) reduction effectiveness along with improving ascorbic acid (AA) stability.

o Both are key components to avoid degradation during HPLC analysis

• Preliminary standard data and processing data for vitamin C before and after retort processing.

3. We have successfully determined optimal retort time for our food matrices addressing high acid and low acid foods

• This information is essential for minimizing vitamin lost during processing to start off with a higher vitamin concentration during storage

• Reference https:// for calculating Fo for low acid foods

4. We optimized our freeze drying protocol for all food matrices to ensure samples are sufficiently dried 5. We have obtained a source for all ingredients to produce in bulk quantities

• Source bulk of ingredients from Springfield Performance Food Group

• Source Strawberries Light in Syrup from Food Service Direct

• Smaller quantity size ingredients will be sourced from local grocery stores

6. We purchased all equipment/supplies needed to make recipes in bulk quantities

• Purchased a convection oven for beef brisket; • Purchased a deli slicer for beef brisket; • Many other equipment/supplies to optimize tasks (e.g., hole puncher, retort pouch holder, lids)

7. We also streamlined each recipe to be able to prepare and retort all samples in one day for each recipe

8. Development and validation of computational model for simulating vitamin degradation in spaceflight foods.

• Isothermal thiamine degradation

The literature indicates that thiamine degradation at storage and accelerated storage temperatures follows first order kinetics. This enabled simplification of our endpoint method to estimate the kinetic parameters from isothermal data. To do the calculations we wrote an interactive Wolfram Demonstration, which is freely downloadable from the Internet (open http://demonstrations.wolfram.com/). This program enables fast estimation of the parameters by manually matching generated degradation curves with two experimental end-concentrations and using them to predict the degradation curves at temperatures not used in the parameters calculation.

The method and program were tested and validated with literature data on thiamine and the results published (See Bibliography below -- Food Research International, 79 (2016), 73-80).

• The successive points method. It has been shown that, at least theoretically, one can extract the parameters of a degradation reaction that follows fixed-order kinetics from two successive concentration ratios determined during non-isothermal storage. The calculation procedure is similar to that of the endpoints method except that a single curve ought to be passed through the two points instead of two – open the interactive freely downloadable Wolfram Demonstration http://demonstrations.wolfram.com/. The method has been tested with computer simulations and with published data on the non-isothermal degradation of vitamin A, see Bibliography below--Food Research International, 75 (2015), 174-181.

• Vitamin C degradation. Examination of the literatures on ascorbic acid degradation revealed that several reported data do not follow the assumed first order kinetics. In some publications this was most probably due to experimental errors. A typical example is that the increasing divergence of the reported degradation curves at different temperatures, which is expected from the Arrhenius equation (or exponential model), was not observed. One report showed that the ascorbic acid's degradation only starts as an exponential decay, which followed first or approximately first order kinetics. Later the decay decelerated and appeared to approach what an asymptotic concentration. This might have been due to the oxygen disappearance, a factor that has not been always adequately monitored let alone or controlled. The problem was less severe in two frozen vegetables (which is consistent with the above suggested explanation). We have written a version of the isothermal endpoints method for frozen foods and intend to make it available as an addition to the already posted Wolfram Demonstration or as a new Demonstration. We will also attempt to modify the degradation model to account for residual concentration of the vitamin. Either way, control or knowledge of the oxygen tension during processing and storage will be essential for the development of a predictive kinetic degradation model. |

• Storage criteria. It has been a common practice to determine a food or pharmaceutical product's shelf life as the time at which the marker's concentration or concentration ratio falls below (or surpasses) a critical concentration. In accelerated storage this time is shortened by the elevated temperature, which shortens the time to reach the set threshold. The question that arises is what happens when there are two markers instead of one, e.g., two vitamins in the same food that follow different degradation kinetics. Computer simulations show that, theoretically, the order in which two different markers cross their corresponding threshold concentrations (in either direction) can but need not always be reversed at different temperatures. In other words, at least in principle, it is possible that the results of accelerated storage experiments will not predict correctly the end of a product's shelf life if determined by a more than a single criterion. The simulation program was posted on the Internet as a freely downloadable interactive Wolfram Demonstration open: (http://demonstrations.wolfram.com/). A detailed discussion of the issue has been published--see Bibliography -- Food Research International, 78 (2015), 388-395. At least theoretically, the same order reversal can happen when there are more than two criteria – open the new Wolfram Demonstration http://demonstrations.wolfram.com/ .

Reference

Ndaw, S.; Bergaentzlé, M.; Aoudé-Werner, D.; Hasselmann, C. Extraction procedures for the liquid chromatographic determination of thiamin, riboflavin and vitamin B6 in foodstuffs. Food Chemistry 2000 Vol. 71 No. 1 pp. 129-138.

Bibliography Type:	Description: (Last Updated: 09/02/2019)
Abstracts for Journals and Proceedings	Peleg M. "A new approach to modeling and predicting vitamins degradation kinetics." Presented at the 2016 NASA Human Research Program Investigators' Workshop, Galveston, TX, February 8-11, 2016. 2016 NASA Human Research Program Investigators' Workshop, Galveston, TX, February 8-11, 2016. Reference ID: 0645-000371 , Feb-2016
Articles in Peer-reviewed Journals	Peleg M, Normand MD. "Predicting chemical degradation during storage from two successive concentration ratios: theoretical investigation." Food Research International. 2015 Sep;75:174-81. http://dx.doi.org/10.1016/j.foodres.2015.06.005 , Sep-2015
Articles in Peer-reviewed Journals	Peleg M, Normand MD. "Simulating shelf life determination by two simultaneous criteria." Food Research International. 2015 Dec;78:388-95. http://dx.doi.org/10.1016/j.foodres.2015.09.003 , Dec-2015
Articles in Peer-reviewed Journals	Peleg M, Normand MD, Goulette TR. "Calculating the degradation kinetic parameters of thiamine by the isothermal version of the endpoint method." Food Research International. 2016 Jan;79:73-80. http://dx.doi.org/10.1016/j.foodres.2015.12.001 , Jan-2016